

Abstract Submitted
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Molecular dynamics simulations of liquid crystalline ordering in bulk and at interfaces XIAOYU WEI, JUSTIN HOOPER, DMITRY BEDROV, Univ of Utah — The influence of induced polarization interactions in atomistic MD simulations on the thermodynamic and structural properties of 4-Cyano-4'-pentylbiphenyl (5CB) bulk systems have been systematically investigated utilizing both polarizable (POL) and non-polarizable (NP) version of the APPLE&P force field (FF). The predicted densities for the nematic and isotropic phases of 5CB are in excellent agreement with available experimental data. However, the nematic-isotropic transition temperature T_{NI} showed noticeable sensitivity to the details of FF. The NP FF showed a tendency to predict systematically higher T_{NI} (by about 30K) and showed very little sensitivity to modifications of dihedral potential in the biphenyl unit. The POL FF showed a much stronger sensitivity to the details of biphenyl conformational properties and was able to predict T_{NI} at around 313K, which is very close to the experimental T_{NI} of 308K. Using the developed potentials we have also investigated the anchoring of nematic 5CB at the water interface as well as phase behavior and structure of the newly discovered twist-bend nematic phase of CB7CB. Detailed analysis of molecular scale correlations for both systems will be presented and discussed in light of available experimental data.

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